Cyclohexane, 1,2-propadienyl-

Other names:	Cyclohexane, propadienyl-
	1-Cyclohexyl-1,2-propadiene
	Cyclohexylallene
Inchi:	InChI=1S/C9H14/c1-2-6-9-7-4-3-5-8-9/h6,9H,1,3-5,7-8H2
InchiKey:	CQHBBSICMXUMIB-UHFFFAOYSA-N
Formula:	C9H14
SMILES:	C=C=CC1CCCCC1
Mol. weight [g/mol]:	122.21
CAS:	5664-17-5

Physical Properties

Property code	Value	Unit	Source
gf	265.47	kJ/mol	Joback Method
hf	113.44	kJ/mol	Joback Method
hfus	11.75	kJ/mol	Joback Method
hvap	35.82	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.908		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
tb	424.82	K	Joback Method
tc	641.76	K	Joback Method
tf	203.32	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.50	J/mol×K	424.82	Joback Method
cpg	245.82	J/mol×K	460.98	Joback Method
cpg	262.28	J/mol×K	497.13	Joback Method
cpg	277.89	J/mol×K	533.29	Joback Method
cpg	292.67	J/mol×K	569.44	Joback Method
cpg	306.64	J/mol×K	605.60	Joback Method

cpg	319.81	J/mol×K	641.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5664175&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume